

# *CENTER FOR CATALYTIC SCIENCE AND TECHNOLOGY*

[www.cbe.udel.edu/ccst](http://www.cbe.udel.edu/ccst)



MAR. 14, 2024 | 2:00 PM | 322 HARKER ISE LAB

**FERNANDO LIMA**

Associate Professor

WEST VIRGINIA UNIVERSITY



## *A PROCESS SYSTEMS FRAMEWORK FOR DESIGN, OPTIMIZATION AND CONTROL OF MODULAR ENERGY SYSTEMS*

This presentation will focus on the development of a process systems framework to enable the design and operations of modular energy systems. Specifically, a novel operability-based approach for process design and intensification of nonlinear energy processes will be introduced, toward facilitating the realization of the concept of modular manufacturing. The developed operability methods are based on nonlinear optimization and computational geometry concepts and explore the nonlinear process mapping relationships between key input/design and output variables. To address the dimensionality challenge that may arise due to process complexity, the incorporation of bilevel and parallel programming approaches as well as machine learning-based methods into the classical process operability concepts will be discussed.

For the operation of modular systems under uncertainties, the interface between the design and control tasks is analyzed. In particular, a dynamic operability mapping is developed to find a feasible region for advanced control applications. To perform the operability mapping computations, a Python-based open-source software package is introduced. This package opens an avenue for collaborations between process systems engineering researchers and others in communities that would benefit from direct/inverse mapping calculations, such as in computational catalysis and materials science. The implementation of the framework to address natural gas utilization examples will be presented, including a catalytic membrane reactor system for the direct methane aromatization conversion to hydrogen and benzene and a natural gas combined cycle plant for power generation.